



FLAGSHIP INITIATIVE  
ENGINEERING  
MOLECULAR SYSTEMS



UNIVERSITÄT  
HEIDELBERG  
ZUKUNFT  
SEIT 1386

# COLLOQUIUM ENGINEERING MOLECULAR SYSTEMS - IN PERSON -

**GANNA GRÝNOVA** will talk about **ENGINEERING ORGANIC FRAMEWORKS FOR MOLECULAR STORAGE** in the “Engineering Molecular Systems” colloquium on **April 24<sup>th</sup> 2023** at **5 p.m.** (CET) hosted by the Flagship Initiative Engineering Molecular Systems of Heidelberg University. The colloquium will take place at the IMSEAM (seminar room 01.413) Im Neuenheimer Feld 225, 69120 Heidelberg.



**Ganna Grynova**  
Computational Carbon  
Chemistry  
HITS Heidelberg

**April 24<sup>th</sup> 2023**  
**5 pm CET**

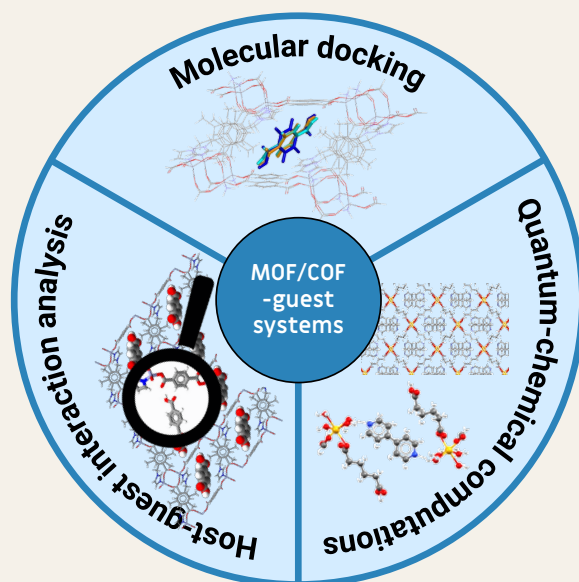
**IMSEAM**  
**Im Neuenheimer Feld 225**  
**seminar room 01.413**



## ABSTRACT:

Organic frameworks are porous crystalline materials that (i) consist of regularly connected nodes and linkers, (ii) have high internal surface areas and low densities, and (iii) can host small guest molecules. Depending on their composition, two principal types of frameworks exist: metal-organic frameworks (MOFs) – which were pioneered by Omar Yaghi in the late 1990s – and the more recently developed covalent-organic frameworks (COFs). Due to their highly tuneable composition, their adaptable structures, and their ability both to absorb and store small guest molecules in their pores and to release these molecules depending on the chemical environment, MOFs and COFs are increasingly often utilised for gas storage and separation, drug delivery, and catalysis.

While accurate structural data are key to unveiling the host-guest interactions in the COF and MOF complexes with their molecular targets, experimental characterisation of these interactions remains rather challenging. In this talk, I will discuss our efforts towards affordable and insightful *in silico* description of the host-guest interactions in organic framework materials and demonstrate how this information can be used to guide their rational targeted design. I will highlight the methodological tips and tricks for locating the stable host-guest complex geometries using multiscale approaches, analysing the noncovalent interactions in them by means of diverse wavefunction- and density-partitioning schemes, and computing the interaction energies at an optimal ratio of accuracy and computational cost.



## REFERENCES

1. M. Ernst, G. Gryn'ova "Engineering Host-Guest Interactions in Organic Framework Materials for Drug Delivery", *under review*, **2023** (preprint DOI: 10.26434/chemrxiv-2023-1f181).
2. M. Ernst, T. Poręba, L. Gnägi, G. Gryn'ova, "Locating Guest Molecules inside Metal–Organic Framework Pores with a Multilevel Computational Approach", *J. Phys. Chem. C*, **2023**, *127*, 523-531.
3. M. Ernst, G. Gryn'ova, "Strength and Nature of Host-Guest Interactions in Metal-Organic Frameworks from a Quantum-Chemical Perspective", *ChemPhysChem* **2022**, *23*, e202200098.



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## **BRIEF CV:**

Apr 2019-present: **Junior Group Leader** “Computational Carbon Chemistry” (CCC) at Heidelberg Institute for Theoretical Studies (HITS gGmbH) and Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University

Nov 2016-Jan 2019: **Marie Skłodowska-Curie Actions Research Fellow**, Institute of Chemical Sciences and Engineering, École polytechnique fédérale de Lausanne (Switzerland)

Nov 2014-Oct 2016: **Postdoctoral Research Fellow**, Institute of Chemical Sciences and Engineering, École polytechnique fédérale de Lausanne (Switzerland)

Sept 2013-Sept 2014: **Postdoctoral Research Fellow**, Research School of Chemistry, Australian National University (Australia)

2010-2013: **PhD** (awarded July 18, 2014), Research School of Chemistry, Australian National University (Australia)

2008-2009: **Master of Science** and tertiary teaching, Department of Chemistry, Oles Honchar Dnipro National University (Ukraine) Diploma with Honours (summa cum laude)

2004-2008: **Bachelor of Science**, Department of Chemistry, Oles Honchar Dnipro National University (Ukraine) Diploma with Honours (summa cum laude)